Antiferromagnetism and phase separation in the *t-J* model at low doping: A variational study

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Using Gutzwiller-projected wave functions, I estimate the ground-state energy of the *t-J* model for several variational states relevant for high-temperature cuprate superconductors. The results indicate that both the superconducting state and the staggered-flux normal state (proposed for vortex cores) are unstable at low doping towards antiferromagnetism and towards phase separation. While phase separation in the underdoped superconducting state may be relevant for the stripe formation mechanism, the results for the normal state suggest that similar charge inhomogeneities may also appear in vortex cores up to relatively high doping values.

After many years of research, the issues of antiferromagnetism and of phase separation in weakly-doped high-T_c cuprates are far from being settled. While it is generally accepted that short-range antiferromagnetic (AF) correlations are crucial for the superconductivity in cuprates, it is not clear whether the long-range antiferromagnetism at very low doping should be considered as a competing order on equal footing with the superconductivity or simply as a minor side effect. The latter point of view is implicitly assumed in the resonating-valence-bond (RVB) scenario of high-temperature superconductivity.[1] In terms of ground-state properties, the RVB approach may be recast into the language of variational Gutzwiller-projected (GP) wave functions.[2–4] Recently considerable progress has been reported in describing properties of high-temperature superconductors with the help of GP wave functions for the Hubbard model in the strong-coupling limit.[5] Most studies of the GP wave functions neglect the long-range AF ordering at low doping, and the resulting phase diagram contains the superconducting phase starting from zero doping. However, it is very easy to take AF order into account by explicitly including it in the variational wave function. Within this approach, the GP wave function for the *t-J* model is known to be energetically unstable with respect to the AF order below the level of doping about 10% (at $J/t=0.3$) (Ref. 6) (see also Ref. 7 for an earlier study).

The phase-separation issue is a much more delicate subject than antiferromagnetism: it is not decided even at the level of the *t-J* model. While the phase separation at large J/t is well established, different studies do not agree about whether the phase separation occurs in the physically relevant parameter range (at $J/t \sim 0.3$).[8–12]

In this work I refine the numerical results of Ref. 6 on the ground-state energy of the superconducting state in presence of AF order and perform a similar analysis for the staggered-flux state recently proposed to describe the normal state in the vortex cores.[13,14] For both normal and superconducting states we find antiferromagnetism and phase separation at low doping. The phase separation follows from the upward convexity of the ground-state energy as a function of doping. Within our approximation, the phase separation persists to higher dopings than antiferromagnetism. Consequently, the coexistence of AF order and superconductivity is not realized as a homogeneous state (at least, for the considered dimen-

sionless parameter $t/J=3$). Instead, at dopings lower than the phase-separation point x_{sep}, it is energetically favorable to split into two phases: the undoped antiferromagnet (with the long-range AF order but without superconductivity) and the superconductor with the doping x_{sep} (without the AF order). The relative areas of the two domains are fixed by the average doping, and the actual shape of the domains is determined by the Coulomb interaction at large distances (neglected at the level of the *t-J* model). This is the phase-separation scenario of the stripe formation.[15–17] Some numerical studies suggest an alternative point of view that stripes appear already in the *t-J* model without any long-range interactions.[18] The results reported in this paper do not have any implications on the latter scenario, since I do not consider here any incommensurate spin-charge-density-wave states. *A priori* it is possible that stripe states with energies lower than the states studied here exist and may also be constructed variationally by Gutzwiller projection.

Regarding the effect of the long-range Coulomb interaction, I only remark that already nearest-neighbor repulsion may act to reduce the phase separation. With increasing nearest-neighbor repulsion, the phase-separation region shrinks to smaller doping values and practically disappears at the repulsion strength about 3-4*J*— approximately equal to the repulsion strength required to suppress superconductivity. (Note that nearest-neighbor repulsion may also favor stripe-like states not considered here.)

Finally, I comment on a similar phase-separation feature in the staggered-flux normal state proposed recently to describe the normal state in the vortex core.[13,14] The phase separation in the normal state appears more prominent and extends to higher doping values than in the superconducting state. This suggests that charge inhomogeneities (an analog of stripes) may also appear in the vortex core. However, as estimated in Ref. 14, the core size should be of order of several lattice spacings, and large gradients of the order parameter play an important role in determining the structure of the core, together with the long-range Coulomb interaction. Thus the problem of the vortex core structure, even at the level of optimizing the Gutzwiller-projected wave function, becomes a very complicated one, and our present analysis of uniform states is not sufficient for solving it. We note here that insulating and antiferromagnetic regions in the vortex

cores have also been predicted in other approaches: in the SO(5) theory[19] and in the unrestricted mean-field analysis.[20]

In the rest of the paper, I present the details of our numeric analysis of the Gutzwiller-projected wave functions.

The variational wave functions studied in this work are chosen to minimize the energy of the t-J Hamiltonian

$$H = P_G \left[\sum_{ij} \left(-t c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.} + J \left(\mathbf{S}_i \mathbf{S}_j - \tfrac{1}{4} n_i n_j \right) \right) \right] P_G, \quad (1)$$

where the sum is taken over the pairs of nearest-neighboring sites i and j on the two-dimensional square lattice, n_i denotes the hole density at a given site. Following the usual Gutzwiller-projection approach, we consider the variational wave functions of the form $\Psi_{GP} = P_G \Psi_0$. Both here and in the Hamiltonian (1) P_G denotes the "double" projection: it projects out components with doubly occupied sites (the usual Gutzwiller projection) and further it also fixes the total number of particles to the required value. Ψ_0 is the ground state of the auxiliary ("mean-field") BCS Hamiltonian

$$H_{\text{BCS}} = \sum_{ij} \left(-\chi_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \Delta_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger) + \text{h.c.} \right)$$
$$+ \sum_i (-1)^i h \sigma_i^z, \quad (2)$$

where $\sigma_i^z = c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}$ is the z-magnetization at site i. We start our variational study with the usual nearest-neighbor d-wave ansatz: $\chi_{ij} = \chi$ on nearest-neighbor links, $\chi_{ii} = \mu$ is the on-site chemical potential, $\Delta_{ij} = \pm \Delta$, with $\pm$ for vertical and horizontal nearest-neighbor links, respectively. Within this variational ansatz, the wave function depends on the three dimensionless parameters: Δ/χ, μ/χ, and h/χ. The parameter h represents an artificial staggered magnetic field acting on spins to produce the long-range AF order. At zero value of h, the minimization has been performed by many authors.[3–5,14] We further adopt the numbers reported in our earlier publication Ref. 14. As in that work, we compute the ground-state energy by the variational Monte Carlo method (see e.g., Ref. 3 for details of the method), on the square lattice 22×22 with the boundary conditions periodic along one direction and antiperiodic along the other direction.[21] For this system size, the finite-size corrections to the ground-state energy are estimated to be of the order of the Monte Carlo statistical errors (about $10^{-3} J$ per site) [in the staggered-flux state the finite-size corrections are somewhat bigger because of the discretization of the Fermi pockets]. The parameter of the t-J model is taken to be $t/J = 3$ throughout the paper.

To check for an instability with respect to the AF ordering, we further minimize the variational energy as a function of h while keeping Δ/χ and μ/χ constant (in principle, the minimization should be performed by varying all the three parameters simultaneously; we can however check that, in the vicinity of the energy minimum, the errors from our simplified minimization procedure are negligible). Instead of characterizing the AF state by the fictitious field h, we use a physically significant quantity, the staggered magnetization. In Fig. 1 we plot the staggered magnetization in the optimal wave function as a function of doping x. We find the insta-
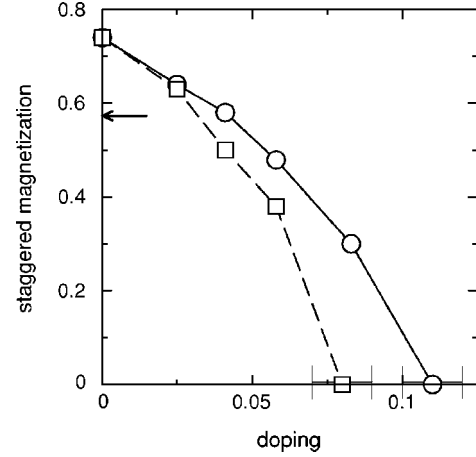

FIG. 1. Staggered magnetization $M = \langle (-1)^i \sigma_i^z \rangle$ as a function of doping at $t/J = 3$ for the superconducting (circles) and staggered-flux (squares) states. Vertical error bars are of the order of the symbol size. Error bars of the phase transition points are about 0.01 (shown). Our results for the superconducting state agree with those in Fig. 2 of Ref. 6. The arrow shows the exact value ($M = 0.60$) of the staggered magnetization in the undoped Heisenberg antiferromagnet.

bility towards the AF ordering below $x_{\text{AF}} = 0.11$. So far the computations repeat those in Ref. 6. Thus obtained values of staggered magnetization should only be considered as an indication of the antiferromagnetic ordering, and not as good numerical estimates of the actual staggered magnetization in the ground state: for example, in the undoped case, the variational estimate is much higher than the known exact value.[22]

If we analyze the resulting ground-state energy as a function of doping, we observe that it is upward convex at low doping. This implies that at those dopings phase separation occurs. In Fig. 2 we plot the ground-state energy with the subtracted linear part $E - \mu_{\text{sep}} x$ as a function of doping. The slope μ_{sep} of the limiting tangent line gives the chemical potential at the phase separation point. The point of contact determines the critical doping x_{sep} below which the phase separation occurs. At $t/J = 3$, we estimate $x_{\text{sep}} = 0.13$ and $\mu_{\text{sep}} = -5.65 J$ (this value of x_{sep} agrees with the estimates of Ref. 10).

Note that for the t-J model with $t/J = 3$ we obtain $x_{\text{sep}} > x_{\text{AF}}$, i.e., a uniform admixture of antiferromagnetism in the superconducting state is always unstable towards phase separation; the phase separation occurs between the undoped antiferromagnet and the superconductor at doping x_{sep} without antiferromagnetism. However, this inequality appears to be nonuniversal, and could, in principle, be reversed by adding other terms like next-nearest-neighbor hopping or nearest-neighbor repulsion (see the discussion of nearest-neighbor repulsion below).

We may further perform the same steps as above for the "normal" staggered-flux (SF) state proposed to describe vortex cores in the mixed state.[13,14] The SF state is characterized by $\Delta_{ij} = 0$, $\chi_{ij} = e^{ia_{ij}}$ for nearest neighbors i and j, $\chi_{ii} = \mu$ is the on-site chemical potential. The vector potential a_{ij} produces a checkerboard pattern of the flux. The value of the flux is a variational parameter, and the chemical-potential parameter
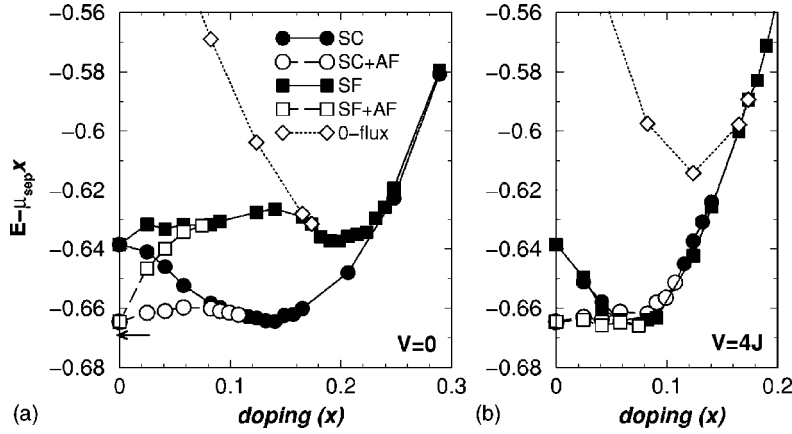
FIG. 2. Energies of different GP wave functions with linear part subtracted ($E-\mu_{sep}x$) as a function of doping x. The five different variational wave functions are compared (optimized in energy within each class): superconducting without antiferromagnetism (solid circles, solid line), superconducting with antiferromagnetism (empty circles, dashed line), staggered-flux without antiferromagnetism (solid squares, solid line), staggered-flux with antiferromagnetism (empty squares, dashed line), and zero-flux (projected Fermi sea, empty diamonds, dotted line). Left panel (a) shows energies in the absence of NN repulsion ($V=0$), with $\mu_{sep}=-5.65$. Right panel (b) corresponds to $V=4J$, with $\mu_{sep}=-4.85$ [NN repulsion is included at the perturbation level via (3)]. The energies are in the units of J per lattice site. Error bars are smaller than the symbol size. For comparison, the arrow in panel (a) shows the exact ground-state energy in the undoped case ($E=-0.669J$) (Ref. 22).

μ is fixed to produce the required doping level.

We first test the SF state for the AF instability and find that, similarly to the superconducting state, the SF state favors AF order at very low doping. We find that the corresponding staggered magnetization (also plotted in Fig. 1) is smaller than in the superconducting state at the same doping. The critical value of doping $x_{AF}^{(SF)}$ is also smaller than in the superconducting state [we estimate $x_{AF}^{(SF)}=0.08$]. Thus antiferromagnetism in vortex cores appears at the first glance more fragile than in the bulk of the superconductor.

However the phase-separation effect in the SF state is more pronounced than in the superconducting state: we estimate $x_{AF}^{(SF)}=0.21$— far in the "overdoped" region of the phase diagram. We summarize our results on the ground-state energies of different states in Fig. 2 (the difference between the energies of the superconducting and SF states was reported previously in Ref. 14 as the condensation energy for the superconducting state). Our results on the phase separation in the SF state indicate that charge inhomogeneities (similar to stripes in underdoped cuprates) are likely to form in the vortex cores up to rather high doping values. As in the case with stripes, the actual structure of inhomogeneities should be determined by the long-range Coulomb interactions. Such inhomogeneities may play a role in producing the "subgap state" features observed in the density of states in the STM experiments.[23]

As a simplified version of long-range Coulomb interaction, we consider the effect of nearest-neighbor (NN) repulsion on the phase separation. The NN repulsion is included as the additional term in the Hamiltonian (1), $H_V=V\Sigma_{ij}n_in_j$, where the sum is taken over all NN pairs of sites [n_i denotes the hole density, as before; V is the repulsion strength in addition to the attraction $-J/4$ already present in the Hamiltonian (1)]. If we neglect the interaction between holes, H_V might be thought to scale as x^2 with doping x. Then a small repulsion energy V might be already sufficient to change the convexity of the total energy as a function of doping and hence to suppress phase separation. In reality, in the superconducting antiferromagnetic state at small doping, the attraction between holes is quite strong, and scaling of H_V with doping is closer to x than to x^2. In Figs. 3(a) and 3(b) we plot the nearest-neighbor correlation function $\langle n_in_j\rangle$ normalized by x and by x^2, respectively (at $V=0$).
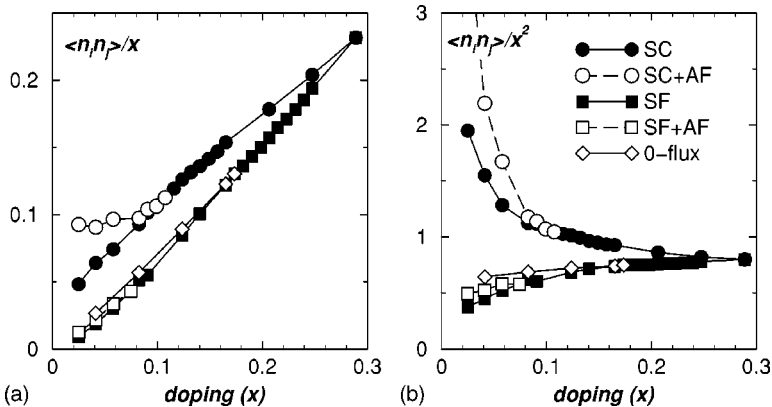

FIG. 3. Nearest-neighbor correlation of the hole density $\langle n_in_j\rangle$ as a function of doping for the same wave functions as in Fig. 2(a) (at $V=0$). Panel (a) shows nearest-neighbor correlation divided by the average hole density x, and in panel (b) the same correlation is divided by x^2.

To roughly estimate the effect of NN repulsion, we approximate the ground-state energy with repulsion as

$$E(x) = E_0(x) + 2V\langle n_i n_j \rangle, \quad (3)$$

where $E_0(x)$ is the variational ground-state energy without repulsion, and the average is taken over the variational ground state without repulsion. In this approximation, we can estimate the repulsion strength necessary to reverse the convexity of the ground-state energy $E(x)$. With increasing the NN repulsion strength V, the upward convexity of the ground-state energy diminishes, and the phase-separation point x_{sep} shifts towards smaller doping (both in the superconducting and the SF states). At the same time, the superconductivity gets also strongly reduced (at least in its present nearest-neighbor d-wave ansatz), with the superconducting transition point shifting to smaller doping. The antiferromagnetism at finite doping is also reduced, but not so strongly as the superconductivity.

With increasing the NN repulsion strength V, the phase separation eventually becomes undetectable within our numerical errors at $V \sim 3-4J$. At the same time, at the repulsion strength of about $4J$, our superconducting wave function loses the energy competition to the staggered-flux one: the price of nearest-neighbor holes overweighs the energy gain from the superconductivity. It is possible however that at such strong NN repulsion another superconducting ansatz (e.g., involving next-nearest-neighbor pairing) would be more energetically favorable (search for such states goes beyond the scope of the present paper). We illustrate the effect of NN repulsion in Fig. 2(b), where the marginal situation is shown: the superconducting state is nearly equal in energy to the SF state at $V=4J$ [with NN repulsion taken into account only to the lowest order in the perturbation theory (3)]. Note

that our numerical results show a rather flat doping dependence of the ground-state energy at very low doping, and this leaves unresolved the issue of whether phase separation at infinitesimally small doping may survive arbitrarily strong NN repulsion. Of course, the above treatment of the hole interaction is only a rough estimate. As suggested in Ref. 24, the variational wave function may be further improved by including additional Jastrow-type factors. Such a modification of the wave function apparently affects the hole-hole correlations,[24] and may therefore be important for a proper assessment of the effects of the hole-hole interaction.

The variational study reported in this paper should be taken with care when applied to actual cuprate superconductors: the phase-separation effect in the superconducting state is weak, and many additional factors may change the picture outlined here.[25] However, I believe that some qualitative conclusions may withstand small perturbations of the model: (1) staggered-flux state is more disposed to phase separation than the superconducting state. This may produce charge inhomogeneities inside the vortex cores; (2) antiferromagnetic ordering at low doping enhances phase separation (this may be a general property of phase separation in doped Mott insulators, see, e.g., Ref. 26, and references therein); (3) both in the staggered-flux state and in the superconducting state, the long-range antiferromagnetic ordering occurs only at low doping (below ~ 0.1). Thus static AF order in vortex cores,[27] if confirmed, possibly indicates regions with reduced hole concentration.

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